TRIM.FaTE USER'S GUIDE MODULE 9: SCENARIO PROPERTIES

This module provides guidance on the scenario properties of a TRIM.FaTE scenario. The information in this module is divided into three sections (plus references):

- (1) A description of the role of TRIM.FaTE scenario properties;
- (2) Instructions on how to set scenario properties; and
- (3) A summary of the scenario properties created by default for a TRIM.FaTE scenario.

1. ROLE OF SCENARIO PROPERTIES

Scenario properties – set by the user on the Scenario view – can be used to direct the way the TRIM.FaTE model executes a given scenario. These properties set the general modeling parameters that define how the model calculates, stores, and presents results. In general, many scenario properties are not included in the current TRIM.FaTE public reference library; instead, they are "built in" to the model and created by default with a new scenario. Other properties can be added to the scenario from a library if desired.

For the current public reference library, some other properties (e.g., *isDay* properties that control exchange via plant stomata, or meteorological properties such as air temperature and wind speed) are defined as scenario properties. However, these properties are not "hard-wired" into the model and do not necessarily need to be set as scenario properties; for example, meteorological properties could be set as properties of volume elements if the appropriate changes were made to the algorithms in the library that reference these properties. This approach would allow the use of multiple sets of meteorological data (e.g., from multiple stations) within the modeling study area. Meteorological properties are explained in detail in Module 10 and are not discussed in the remainder of this module.

2. SETTING SCENARIO PROPERTIES

Scenario property values can be set by the user on the Scenario view within the Scenario window (see Figure 1). Properties can be edited directly in the Property Editor on the right side of the view. To edit a value, double-click the cell to be edited, delete the existing value, and type in the new value. Remember to push the "Enter" key after changing the value (if Enter is not pushed, the change will not be saved in the scenario).

Alternatively, scenario properties can be included in a Property Import file and imported as a part of the scenario set-up process. For example, a section of the Property Import file that contains the scenario properties for averaging interval, output directory, and simulation begin and end dates and times would be formatted as follows:

Scenario: TestSite Property: averagingInterval Value: monthly Property: outputDir Value: \\Models\\TRIM\\data\\results\\TestSite
Property: simulationBeginDateTime
Value: 01/01/1990 00:00:00 EST
Property: simulationEndDateTime
Value: 12/31/1995 22:00:00 EST

Refer to Module 3, Library and Scenario Data Files, for formatting requirements for the Property Import file and detailed instructions on how to set up and use this file.

USER TIPS: SETTING THE SCENARIO PROPERTIES

- If an HTML output file is to be created, make sure the designated date for an HTML export (i.e., the property *evaluateHTMLPropertiesAtTime*) is set within the scenario start/end dates. Setting this date outside of the start/end dates will lead to an error during scenario verification.
- In general, all scenario properties must be assigned values by the user before attempting to verify a scenario. Exceptions include *averagingInterval* and *evaluateHTMLProperties AtTime*, which can remain "<Unset>" in some instances (see Table 1 for details).
- ► The user can instruct TRIM.FaTE to automatically average results by setting the scenario property AverageResultsFiles to true. The model would then calculate a mathematical average for each output value for the time period (e.g., every 4 hours, monthly) specified by the user with the scenario property AveragingInterval. Alternatively, the user could perform these averaging calculations manually after the run is completed using the Averager tool or tools external to TRIM.FaTE.

👸 FaTE Scenario: SampleScenario				_ 8 ×				
File Edit <u>A</u> dd <u>R</u> un View Help								
Scenario Sources Chemicals Compartments Links Algorit	hms Analyses							
Project: SampleScenario Properties								
New Del Ref PTyne Form Show All Linda Reda								
			[
	Property Name	Value	Units	Data				
1	AirTemperature_K	C:Wodels\TRIM\data\SampleScenario\Met\	degrees K	Real Numbe				
2	averageResultsFiles	true		True or Fal:				
3	averagingInterval	annual		Text				
4	CumulativeRain	0.0	m	Real Numbe				
5	dynSimAbsoluteTolerance	1.0E-12	N/A	Real Numbe				
6	dynSimMaxSolverIterations	30000	N/A	Integer				
7	dynSimRelativeTolerance	1.0E-10	N/A	Real Numbe				
8	elasticityThreshold	0.01	N/A	Real Numbe				
9	enableBoundaryContributions	true		True or Fal:				
10	evaluateHTMLPropertiesAtTi	07/04/2000 12:00:00 EST		Date and Ti				
11	exportAllResultsToDB	false		True or Fal:				
12	exportAvgResultsToDB	false		True or Fal:				
13	exportBiotaIntakeRates	true		True or Fal:				
14	exportConcentration	true		True or Fal:				
15	exportDeposition	false		True or Fal:				
16	exportHTML	true		True or Fal:				
17	exportIngestionInputs	false		True or Fal:				
18	exportMass	true		True or Fal				
19	exportMoles	true		True or Fals				
Derived From:				•				
	•							

Figure 1 Scenario View

3. SUMMARY OF SCENARIO PROPERTIES

The scenario properties created by TRIM.FaTE with the creation of a new scenario are described in Table $1.^{1}$

Property Name	Type of Data	Description
appendNumberToRun	true/false	When this value is true, TRIM.FaTE appends a number (e.g., 0, 1, 2) to the end of each output file name. This option prevents the model from writing over the output files of a previous simulation within the current session. However, once the model has been shut down and restarted, TRIM.FaTE may overwrite previous output files. This property is not included in the Scenario window by default, and thus it must be added if the user wants to use a value other than the default of "true."
averageResultsFiles	true/false	If this property is true TRIM will automatically average your results files after a TRIM.FaTE simulation has completed using the averaging period that the user specifies with the <i>averagingInterval</i> property .
averagingInterval	real number (integer), or "monthly" or "annual"	An integer specifying the number of hours to average in the results files (could also be 'monthly' or 'annual'). Although this property is always included in the scenario, the user can leave it as <unset> if they set <i>averageResultsFiles</i> to "false."</unset>
dynSimAbsoluteTolerance	real number	When <i>simulateSteadyState</i> is false, the absolute error tolerance for the differential equation solver.
dynSimMaxSolverIterations	real number (integer)	When <i>simulateSteadyState</i> is false, the maximum number of iterations the differential equation solver should use before giving up.
dynSimRelativeTolerance	real number	When <i>simulateSteadyState</i> is false, the relative error tolerance for the differential equation solver.
elasticityThreshold	real number	For a sensitivity analysis, the elasticity below which the sensitivity results should be set to 0. Elasticity is the percent change in output divided by the percent change in input. If a property has a small elasticity, it can still sometimes cause a false positive and show up as an important parameter, but the elasticity indicates how much relative change resulted from that parameter.
enableBoundaryContributions	true/false	When this is true, TRIM.FaTE will take into account the <i>BoundaryContribution</i> properties defined for compartments; otherwise, it will ignore this property and not include any boundary sources.
evaluateHTMLPropertiesAt Time	date and time (mm/dd/yyyy HH:MM:SS TimeZone)	The date/time at which the values of properties should be evaluated in the HTML export. Although this property is always included in the scenario, the user can leave it as <unset> if <i>exportHTML</i> is set to "false."</unset>

Table 1Scenario Properties

¹When needed, additional properties can be added to the scenario by the user using the "New" button in the Scenario view of the Scenario window.

Property Name	Type of Data	Description
exportAllResultstoDatabase	true/false	When this value is true, the raw data (i.e., the outputs at the output time steps) from FaTE are exported to the output data files (only applies if <i>exportIngestionInputs</i> or <i>exportRiskECOInputs</i> is true).
exportAvgResultstoDatabase	true/false	When this value is true, the averaged data files (i.e., the outputs at the <i>averagingIntervals</i>) from FaTE are exported to the output data files (only applies if <i>exportIngestionInputs</i> or <i>exportRiskECOInputs</i> is true).
exportBiotaIntakeRates	true/false	When this value is true, the intake rate files for biota used by the TRIM.Risk-Eco module are output at the end of the simulation.
exportConcentration	true/false	When this value is true, the results are output in concentration units.
exportDeposition	true/false	When this value is true, the four deposition values (wet particle, dry particle, wet vapor, and dry vapor) are exported (in units of $g/day-m^2$) to the output data files.
exportHTML	true/false	When this value is true, the HTML export for the point in time specified by the <i>evaluateHTMLPropertiesAtTime</i> property is created after the FaTE simulation has completed.
exportIngestionInputs	true/false	When this value is true, the inputs needed for the Expo/Ingestion module are exported to the FaTE output data files.
exportMass	true/false	When this value is true, mass results files are generated for the scenario.
exportMoles	true/false	When this value is true, moles results files are generated for the scenario.
exportOutdoorEnvironment BeforeRun	true/false	When this value is true, an Outdoor Environmental Export is automatically performed when a simulation is run.
exportPropertiesBeforeRun	true/false	When this value is true, a Scenario Property Export is automatically performed prior to the simulation.
exportRiskECOInputs	true/false	When this value is true, the inputs needed for the Risk/Eco module are exported to the FaTE output data files.
exportTimeStepsDown	true/false	When this value is true, the time steps (as opposed to the compartments) will be listed down the leftmost column of the results files.
fateVersion	text	Indicates the version of the TRIM.FaTE model that is currently being run; this property allows the version number to appear in HTML and property exports.
FractionInitialConcentration	real number	The fraction of the initial concentrations in each compartment to be included in the simulation.
mySQLDataDir	directory (e.g., c:\mysql\data)	The full path to the data directory used by MySQL.
outputDir	directory (e.g., c:\data\results)	Indicates the directory where Simulation output data files should be written.
Run_ID	[set by TRIM]	The Run_ID for the current simulation. This value is set automatically by the model at run time (i.e., the user does not need to specify the value).

Property Name	Type of Data	Description
significantDigits	real number (integer)	The number of significant digits to use when writing results to a file. For example, a value of 4 would cause results to have the form 9.999E9.
simulateSteadyState	true/false	Directs the model to perform a steady state simulation (if true) or time-varying simulation (if false).
simulationBeginDateTime	date/time (mm/dd/yyyy HH:MM:SS TimeZone)	The date and time at which a time-varying simulation should begin.
simulationEndDateTime	date/time (mm/dd/yyyy HH:MM:SS TimeZone)	The date and time at which a time-varying simulation should end, inclusive.
simulationStepsPerOutput Step ^a	real number (integer)	The number of simulation time steps in each output time step (simulation results will be output only at each output time step). To output results at each simulation time step, set this value to 1.
simulationTimeStep ^a	real number (integer)	The duration (in hours) of each simulation time step.
steadySimAbsoluteTolerance	real number	When <i>simulateSteadyState</i> is true, the absolute error tolerance for the linear equation solver.
steadySimMaxSolver Iterations	real number (integer)	When <i>simulateSteadyState</i> is true, the maximum number of iterations the linear equation solver should use before giving up.
steadySimRelaxationParam	real number	When <i>simulateSteadyState</i> is true, the relaxation parameter for the Jacobi linear equation solver.
timeZoneForResults	time zone (e.g., EST)	The time zone for which to output the simulation results.

^a Refer to Volume I of the TRIM.FaTE Technical Support Document (EPA 2002) for more details on setting these time-related properties.

4. **REFERENCES**

U.S. Environmental Protection Agency. 2002. TRIM.FaTE Technical Support Document. Volume I: Description of Module. EPA-453/R-02-011a. Office of Air Quality Planning and Standards.

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